Exact solution of Schrödinger equation for modified Kratzer's molecular potential with the position-dependent mass

Ramazan Sever [1], Cevdet Tezcan [2]

[1] *Middle East Technical University,Department of Physics, 06531 Ankara, Turkey*

[2]*Faculty of Engineering, Başkent University, Bağlıca Campus, Ankara, Turkey*

February 2, 2008

Abstract

Exact solutions of Schrödinger equation are obtained for the modified Kratzer and the corrected Morse potentials with the position-dependent effective mass. The bound state energy eigenvalues and the corresponding eigenfunctions are calculated for any angular momentum for target potentials. Various forms of point canonical transformations are applied.

PACS numbers: 03.65.-w; 03.65.Ge; 12.39.Fd

Keywords: Morse potential, Kratzer potential, Position-dependent mass, Point canonical transformation, Effective mass Schrödinger equation.

1 Introduction

Solutions of Schrödinger equation for a given potential with any angular momentum have much attention in chemical physics systems. Energy eigenvalues and the corresponding eigenfunctions provide a complete information about the diatomic molecules.

Morse and Kratzer potentials [1,2] are one of the well-known diatomic potentials. The method used in the Schrödinger equation for vibration-rotation states are mostly based on the wave function expansion and exact solution for a single state with some restrictions on the coupling constants [3-7]. On the other hand solutions of the position-dependent effective-mass Schrödinger equation are very interesting chemical potential problem.

They have also found important applications in the fields of material science and condensed matter physics such as semiconductors[8], quantum well and quantum dots[9], ^3H, clusters[10], quantum liquids[11], graded alloys and semiconductor heterostructures]12,13].

Recently, number of exact solutions on these topics increased[14-31]. Various methods are used in the calculations. The point canonical transformations (PCT) is one of these methods providing exact solutions of energy eigenvalues and corresponding eigenfunctions [24-27]. It is also used for solving the Schrödinger equation with position-dependent effective mass for some potentials [8-13].

In the present work, we solve two different potentials with the three mass distributions. The point canonical transformation is taken in the more general form introducing a free parameter. This general form of the transformation will provide us a set of solutions for different values of free parameter. In this work, the exact solution of Schrödinger equation is obtained or the modified Kratzer type of molecular potential [31] and the corrected Morse potential [32].

The contents of the paper is as follows. In section 2, we present briefly the solution of the Schrödinger by using point canonical transformation. In section 3, we introduce some applications for the specific mass distributions. Results are discussed in section 4.

2 Method

To introduce the PCT, we start from a time independent Schrödinger equation for a potential $V(y)$

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(y)\right)\phi(y)=E\phi(y) \tag{1}$$

where the atomic unit $\hbar=1$ and the constant mass $M=1$ are taken. Defining a transformation $y\rightarrow x$ for a mapping $y=f(x)$, the wave function can be rewritten as

$$\phi(y)=m(x)\psi(x). \tag{2}$$

The transformed Schrödinger equation takes

$$\left\{-\frac{1}{2}\frac{d^2}{dx^2}-\left(\frac{m'}{m}-\frac{f''}{2f'}\right)\frac{d}{dx}-\frac{1}{2}\left[\frac{m''}{m'}+(\alpha-1)\left(\frac{m'}{m}\right)^2-\left(\frac{m'}{m}\right)\frac{f''}{f'}\right]\right.$$

$$\left.+\quad (f')^2\ V(f(x))\right\}\ \psi(x)=(f')^2E\ \psi(x), \tag{3}$$

where the prime denotes differentiation with respect to x. On the other hand the one dimensional Schrödinger equation with position dependent mass can be written as

$$-\frac{1}{2}\frac{d}{dx}\left[\frac{1}{M(x)}\frac{d\psi(x)}{dx}\right]+\tilde{V}(x)\psi(x)=\tilde{E}\psi(x), \tag{4}$$

where $M(x)=m_0\ m(x)$, and the dimensionless mass distribution $m(x)$ is real function. For simplicity, we take $m_0=1$. Thus, Eq. (4) takes the form

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+\frac{m'}{2m}\frac{d}{dx}+m\tilde{V}(x)\right)\psi(x)=m\tilde{E}\psi(x). \tag{5}$$

Comparing Eqs. (3) and (5), we get the following identities

$$\frac{f''}{2f'}-\frac{m'}{m}=\frac{m'}{2m} \tag{6}$$

and

$$\tilde{V}(x)-\tilde{E}=\frac{f'^2}{m}\left[V(f(x))-E\right]-\frac{1}{2m}\left[\frac{m''}{m}-\left(\frac{m'}{m}\right)\left(\frac{f''}{f'}\right)\right] \tag{7}$$

From Eq. (6), one gets

$$f'=m^{1/2} \tag{8}$$

Substituting f' into Eq. (7), the new potential can be obtained as

$$\tilde{V}(x)=V(f(x))-\frac{1}{8m}\left[\frac{m''}{m}-\frac{7}{4}\left(\frac{m'}{m}\right)^2\right]. \tag{9}$$

Therefore, the energy eigenvalues and corresponding wave functions for the potential $V(y)$ as E_n and $\phi_n(y)$ become

$$\tilde{E}_n \;=\; E_n \tag{10}$$

and

$$\psi_n(x) \;=\; \frac{1}{m(x)}\phi_n(y) \tag{11}$$

3 Applications

We solve Schrödinger equation exactly for two potentials the rotationally corrected Morse potential[30] and the modified Kratzer molecular potential[31]. We consider three kinds of the position dependent mass distributions. Two of them are used before[19], and the third one is the exponentially decreasing mass distribution with a free parameter q.

3.1 Modified Kratzer Potential

$$V(r) = D_e \left(\frac{y - y_e}{y} \right)^2, \tag{12}$$

where D_e is the dissociation energy and y_e is the equilibrium internuclear separation. Energy spectrum and the wave functions are

$$E_{n\ell}(n) = D_e - \frac{\hbar^2}{2\mu} \left[\left(\frac{4\mu D_e y_e}{\hbar^2} \right)^2 \left(1 + 2n + \sqrt{1 + 4\left(\frac{2\mu D_e y_e^2}{\hbar^2} + \ell(\ell+1) \right)} \right)^{-2} \right], \tag{13}$$

$$R_{n\ell} = A_{n\ell} (2i\varepsilon y)^{-\frac{1}{2}(1-\eta)} e^{-i\varepsilon y} L_n^{\sqrt{1+4\gamma}}(2i\varepsilon y) \tag{14}$$

where

$$\eta = \sqrt{1 + 4\gamma}, \tag{15}$$

$$\gamma = \frac{2\mu \left(D_e y_e^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu} \right)}{\hbar^2}, \tag{16}$$

$$A_{n\ell} = \left(\frac{8\mu D_e y_e}{\hbar^2 (2n + \eta + 1)} \right)^{3/2} \left[\frac{n!}{(2n + \eta + 1)(n + \eta)!} \right]^{1/2}, \tag{17}$$

$$\epsilon = \frac{i\beta}{(2n + \eta + 1)}, \tag{18}$$

and

$$\beta = -\frac{4\mu D_e y_e}{\hbar^2}, \tag{19}$$

3.1.1 Asymptotically vanishing mass distribution $m(x) = \frac{a^2}{q+x^2}$

$$y = f(x) = \int m(x)^{1/2} dx = a\ell n(x + \sqrt{q + x^2}), \tag{20}$$

The target potential is

$$\tilde{V}(x) = D_e \left[\frac{a\ell n(x + \sqrt{q + x^2}) - y_e}{a\ell n(x + \sqrt{q + x^2})} \right]^2 - \frac{1}{8a^2} \frac{2q + x^2}{q + x^2}, \tag{21}$$

Energy eigenvalues and the normalized radial wave function for the target potential $\tilde{V}(x)$ are

$$\tilde{E}_n = E_{n\ell}(n), \tag{22}$$

$$R_{n\ell}(x) = A_{n\ell} (2i\varepsilon \ell n(x + \sqrt{q + x^2}))^{-\frac{1}{2}(1-\eta)} e^{-i\varepsilon \ell n(x + \sqrt{q+x^2})} L_n^{\sqrt{1+4\gamma}}(2ia\varepsilon \ell n(x + \sqrt{q + x^2})) \tag{23}$$

$$A_{n\ell}^2 = \frac{4an!(1 + n + \varepsilon_1)^2 (2\sqrt{\varepsilon_3})^{2\varepsilon_1}}{(1 + n + 2\varepsilon_1)!}. \tag{24}$$

3.1.2 Asymptotically vanishing mass distribution $m(x) = \frac{a^2}{(b+x^2)^2}$

$$y = f(x) = \int m(x)^{1/2} dx = \frac{a}{\sqrt{b}} \tan^{-1} \frac{x}{\sqrt{b}}, \tag{25}$$

The target potential

$$\tilde{V}(x) = D_e \left(\frac{\frac{a}{\sqrt{b}} \tan^{-1} \frac{x}{\sqrt{b}} - y_e}{\frac{a}{\sqrt{b}} \tan^{-1} \frac{x}{\sqrt{b}}} \right)^2 - \frac{1}{2a^2}(b + 2x^2), \tag{26}$$

and the corresponding energy spectrum and the wave function are

$$\tilde{E}_n = E_{n\ell}(n), \tag{27}$$

$$R_{n\ell}(x) = A_{n\ell} \left(2i\varepsilon \frac{a}{\sqrt{b}} \tan^{-1} \frac{x}{\sqrt{b}} \right)^{-\frac{1}{2}(1-\eta)} e^{-i\varepsilon \frac{a}{\sqrt{b}} \tan^{-1} \frac{x}{\sqrt{b}}} L_n^{\sqrt{1+4\gamma}} (2i\varepsilon \frac{a}{\sqrt{b}} \tan^{-1} \frac{x}{\sqrt{b}}). \tag{28}$$

3.1.3 Exponentially vanishing mass distribution $m(x) = e^{-qx}$

$$y = f(x) = \int m(x)^{1/2} dx = -\frac{2}{q} e^{-\frac{q}{2}x}, \tag{29}$$

the target potential

$$\tilde{V}(x) = D_e \left(1 + \frac{1}{2} q r_e e^{\frac{q}{2}x} \right)^2 + \frac{9}{128} q^4 e^{-qx}, \tag{30}$$

and the corresponding energy spectrum and the wave function are

$$\tilde{E}_n = E_{n\ell}(n), \tag{31}$$

$$R_{n\ell}(x) = A_{n\ell} \left(-\frac{4}{\alpha} i\varepsilon e^{-\frac{\alpha}{2}x} \right)^{-\frac{1}{2}(1-\eta)} e^{\frac{2}{\alpha} i\varepsilon e^{-\frac{\alpha}{2}x}} L_n^{\sqrt{1+4\gamma}} (-\frac{4}{\alpha} i\varepsilon e^{-\frac{\alpha}{2}x}). \tag{32}$$

3.2 Rotationally corrected Morse Potential

$$V(y) = D(e^{-2\alpha y} - 2e^{-\alpha y}) + \gamma(D_0 + D_1 e^{-\alpha y} + D_2 e^{-2\alpha y}), \tag{33}$$

$$\alpha = a r_0, \tag{34}$$

$$\gamma = \frac{\hbar^2 \ell(\ell+1)}{2\mu r_0^2}, \tag{35}$$

r_0 is the equilibrium intermolecular distance, a is a parameter controlling the width of the potential wall. D is the dissociation energy and

$$D_0 = 1 - \frac{3}{\alpha} + \frac{3}{\alpha^2}, \tag{36}$$

$$D_1 = \frac{4}{\alpha} - \frac{6}{\alpha^2}, \tag{37}$$

$$D_2 = -\frac{1}{\alpha} + \frac{3}{\alpha^2}, \tag{38}$$

Energy spectrum and the radial wave function are

$$E_{n\ell} = \frac{\hbar^2 \ell(\ell+1)}{2\mu r_0^2}\left(1 - \frac{3}{ar_0} + \frac{3}{a^2 r_0^2}\right) - \frac{\hbar^2 a^2}{2\mu}\left[\frac{\varepsilon_2}{2\sqrt{\varepsilon_3}} - (n+\frac{1}{2})\right]^2, \tag{39}$$

where

$$\frac{\varepsilon_2}{2\sqrt{\varepsilon_3}} = \frac{1}{a^2\sqrt{\varepsilon_3}}\left[\frac{2\mu D}{\hbar^2} - \frac{\ell(\ell+1)}{r_0^2}\left(\frac{2}{ar_0} - \frac{3}{a^2 r_0^2}\right)\right], \tag{40}$$

$$R_{n\ell}(y) = A_{n\ell} e^{-\alpha\varepsilon_1 y} e^{-\sqrt{\varepsilon_3}e^{-\alpha y}} L_n^{1+2\varepsilon_1}(2\sqrt{3}e^{-\alpha y}), \tag{41}$$

$$-\varepsilon_1^2 = \frac{2\mu r_0^2(E_{n\ell} - \gamma D_0)}{\hbar^2\alpha^2}, \tag{42}$$

$$-\varepsilon_2 = \frac{2\mu r_0^2(2D - \gamma D_1)}{\hbar^2\alpha^2}, \tag{43}$$

$$-\varepsilon_3 = \frac{2\mu r_0^2(D + \gamma D_2)}{\hbar^2\alpha^2}, \tag{44}$$

3.2.1 Asymptotically vanishing mass distribution $m(x) = \frac{a^2}{q+x^2}$

y is given in 3.1.1. The target potential

$$\tilde{V}(x) = \frac{D + \gamma D_1}{(x + \sqrt{q+x^2})^{2\alpha a}} + \frac{\gamma D_1 - 2D_2}{(x + \sqrt{q+x^2})^{\alpha a}} + \gamma D_0 \tag{45}$$

Energy spectrum and the wave function are

$$\tilde{E}_n = E_{n\ell}(n), \tag{46}$$

$$R_{n\ell}(x) = \frac{A_{n\ell}}{(x + \sqrt{q+x^2})^{\alpha\varepsilon_1 a}} e^{-\frac{\sqrt{\varepsilon_3}}{(x+\sqrt{q+x^2})^{\alpha a}}} L_n^{1+2\varepsilon_1}\left(\frac{2\sqrt{\varepsilon_3}}{(x + \sqrt{q+x^2})^{\alpha a}}\right). \tag{47}$$

3.2.2 Asymptotically vanishing mass distribution $m(x) = \frac{a^2}{(b+x^2)^2}$

The target potential

$$\tilde{V}(x) = (D + \gamma D_1) e^{-\frac{2\alpha a}{\sqrt{b}}\tan^{-1}\frac{x}{\sqrt{b}}} + (\gamma D_1 - 2D) e^{-\frac{\alpha a}{\sqrt{b}}\tan^{-1}\frac{x}{\sqrt{b}}} + \gamma D_0 - \frac{q + 2x^2}{2a^2} \tag{48}$$

Energy spectrum and the wave function are

$$\tilde{E}_n = E_{n\ell}(n), \tag{49}$$

$$R_{n\ell}(x) = A_{n\ell} e^{-\varepsilon_1 Px} e^{-\sqrt{\varepsilon_3} e^{-Px}} L_n^{1+2\varepsilon_1}\left(2\sqrt{\varepsilon_3}\, e^{-Px}\right). \tag{50}$$

3.2.3 Exponentially vanishing mass distribution $m(x) = e^{-qx}$

The target potential

$$\tilde{V}(x) = D\left(e^{\frac{4\alpha}{q}e^{-\frac{qx}{2}}} - 2e^{\frac{2\alpha}{q}e^{-\frac{qx}{2}}}\right) + \gamma\left(D_0 + D_1 e^{\frac{2\alpha}{q}e^{-\frac{qx}{2}}} + D_2 e^{\frac{4\alpha}{q}e^{-\frac{qx}{2}}}\right), \tag{51}$$

Energy spectrum and the wave function

$$\tilde{E}_n = E_{n\ell}(n), \tag{52}$$

$$R_{n\ell}(x) = A_{n\ell}[T(x)]^{\epsilon_1} e^{-\sqrt{\epsilon_3}T(x)} L_n^{1+2\epsilon_1}\left(2\sqrt{3}T(x)\right) \tag{53}$$

where $T(x) = e^{Q(x)}$ and $Q(x) = \frac{2\alpha}{q}e^{-\frac{q}{2}x}$.

4 Conclusions

We have applied the PCT in a general form by introducing a free parameter to solve the Schrödinger equation for the corrected Morse and modified Kratzer potentials with spatially dependent mass. In the computations, we have used three position dependent mass distributions. Energy eigenvalues and corresponding wave funtions for target potentials are written in the compact form.

5 Acknowledgements

This research was partially supported by the Scientific and Technological Research Council of Turkey.

References

[1] P. M. Morse, Phys. Rev. **34**, 57 (1929).

[2] A. Kratzer, Z. Phys. **3**, 289 (1920).

[3] A. O. Barut, J. Math. Phys. **21**, 568 (1980); A. O. Barut, M. Berrondo, G. Garcia-Calderon, J. Math. Phys. **21**, 1851 (1980).

[4] A. E. DePristo, J. Chem. Phys. **74**, 5037 (1981).

[5] S. Ozcelik, Tr. J. Phys. **20**, 1233 (1996).

[6] M. Znojil, J. Mat. Chem. **26**, 157 (1999).

[7] J. P. Killingbeck, A. Grosjean, G, Jolierd, J. Chem. Phys. **116**, 447 (2002).

[8] Bastard, G. "*Wave Mechanics Applied to Heterostructure*", (Les Ulis, Les Edition de Physique, 1989).

[9] P. Harrison, "*Quantum Wells, Wires and Dots*" (New York,

[10] M. Barranco et al., Phys. Rev. **B56**, 8997 (1997).

[11] F. Arias et al., Phys. Rev. **B50**, 4248 (1997).

[12] C. Weisbuch and B. Vinter "*Quantum Semiconductor Heterostructure*", (New York, Academic Press, 1993) and references therein; O. Von Roos, Phys. Rev. **B27**, 7547 (1983); O. Von Roos and H. Mavromatis, Phys. Rev. **B31**, 2294 (1985); R. A. Morrow, Phys. Rev. **B35**, 8074 (1987); V. Trzeciakowski, Phys. Rev. **B38**, 4322 (1988); I. Galbraith and G. Duygan Phys. Rev. **B38**, 10057 (1988); K. Young, Phys. Rev. **B39**, 13434 (1989); G. T. Einvoll et al., Phys. Rev. **B42**, 3485 (1990); G. T. 1Einvoll, Phys. Rev. **B42**, 3497 (1990).

[13] J. Yu, S. H. Dong, G. H. Sun, Phys. Lett. **A322**, 290 (1999).

[14] S. H. Dong, M. Lozada-Cassou, Phys. Lett. **337**, 313 (2005).

[15] A. D. Alhaidari, Phys. Rev. **A66**, 042116; A. D. Alhaidari, Int. J. Theor. Phys. **42**, 2999 (2003).

[16] B. Gönül, O. Özer, B. Gönül, F. Üzgün, Mod. Phys. Lett. **A1**, 2453 (2002).

[17] J. Yu, S. H. Dong, Phys. Lett. **A325**, 194 (2004).

[18] G. Chen, Z. D. Chen, Phys. Lett. **A331**, 312 (2004).

[19] K. Bencheikh, S. Berkane, S. Bouizane, J. Phys. A: Math. Gen. **37**, 10719 (2004).

[20] R. Koc, H. Tütüncü, Ann. Pjys.(leipzig) **12**, 684 (2003).

[21] L. Dekar, , T. Chetouani, F. Hammann, J. Phys. A: Math. Gen. **39**, 2551 (1998); L. Dekar, , T. Chetouani, F. Hammann, Phys. Rev. **A59**, 107 (1999).

[22] A. R. Plastino, A. Rigo, M. Casas, A. Plastino, Phys. Rev. **A60**, 4318 (1999).

[23] V. Milanović, Z. Ikonić, J. Phys. A: Math. Gen., **32**, 7001 (1999).

[24] A. de S. Dutra, C. A. S. Almeida, Phys. Lett. **A275**, 25 (2000); A. de S. Dutra, , M. B. Hott, C. A. S.Almeida, Europhys. Lett. **62**, 8 (2003).

[25] R. Koc, M. Koca, E. Körcük, E., J. Phys. A: Math. Gen. **35**, L527 (2002); R. Koc, M. Koca, J. Phys. A: Math. Gen. **36**, 8105 (2003).

[26] B. Roy, P. Roy, J. Phys. A: Math. Gen. **36**, 8105 (2003); B. Roy, P. Roy, Phys. Lett. **A340**, 70 (2005).

[27] C. Quesne, V. M. Tkachuk, J. Phys. A: Math. Gen. **37**, 4267 (2004).

[28] Y. C. Ou, Y. C., Z. Q. Cao, Q. H. Shen, J. Phys. A: Math. Gen. **37**, 4283 (2004).

[29] B. Bagchi, et al, Mod. Phys. Lett. **A19**, 2765 (2004); B. Bagchi, et al, Czech. J. Phys. **54**, 1019 (2004); BB. Bagchi, et al, J. Phys. A: Math. Gen. **38**, 2929 (2004).

[30] Z. D. Chen, G. Chen, , Phys. Scrip. **72**, 11 (2005).

[31] C. Berkdemir, A. Berkdemir, J. Han, Chem. Phys. Lett. **417**, 326 (2006).

[32] C. Berkdemir, J. Han, Chem. Phys. Lett. **409**, 203 (2006).

[33] S. H. Dong, G. H. Sun, Phys. Lett. **314**, 261(2005).

[34] L. Jiang, L. Z. Yi, , C. S. Jia, Phys. Lett. **A345**, 279 (2005).